It's time to select a final project. Pick either the problem set problem or the computational project. Please let me know what you're choosing to do next Tuesday.

1. **A multi-part problem set question.**

   One option is to write a detailed multi-part problem set question in the style of the problems you've been solving for this class. **If you choose this option, I want you to select a topic that you feel you don't really understand fully.** Your topic could be something that is considered elementary but that you think your new stat mech training will help you appreciate on a deeper level (something like our ideal gas law problem, for example). Or you can of course take on a more advanced topic. Things that will be useful for your research are definitely allowed! The one thing I don't want is for you to pick a topic that you're already really familiar with. For example, I don't want someone who has taken a lot of chemical engineering thermodynamics courses writing a problem on the Carnot heat engine. I'm asking you to submit your choice on Tuesday, November 20 so we have time to discuss it and make sure that you're really picking something that will be a reasonable challenge for you. To get you thinking of options, here is a (non-exhaustive) list:

   - Ideal solutions and chemical potential. Why does the chemical potential in a dilute solution vary with the logarithm of the concentration?
   - The Nernst equation and electrochemistry. Seriously, what's up with redox reactions? What do we mean by an electrochemical potential and why does it have to do with concentrations of the redox species?
   - Free energy of binding. How does the probability of a ligand binding to a protein relate to the equilibrium constant and to the work required to remove the ligand?
   - Legendre transforms in statistical mechanics and in thermodynamics. These tend to be much more foreign than Laplace or Fourier transforms. What's up with them? Why do they pop up? How do you use them? Can you numerically implement them?
   - Heat engines. We talked about reversible transformations as those where you'd get back all the work you put into them when you reversed the process. Yet Carnot and Stirling heat engines carry out reversible transformation in a cycle to actually perform useful work. What's up with that?!
   - Identical particles and indistinguishability. There are notoriously tricky problems with indistinguishability of particles and quantum mechanics as well as in the classical limits. You could write a problem to explore this. If you're really ambitious, you could discuss ortho/para hydrogen.
   - Heat capacity and low temperature crystals. Debye and Einstein had different models to try to understand the microscopic motions of crystals at low temperatures. One of them got it right.
   - Molecular dynamics and the Verlet algorithm. How does one carry out Newton's laws in a computer? What is up with symplectic algorithms? The volume of phase space? What size of time step is too big?
   - Overdamped Langevin/Brownian dynamics. How do you pass from a deterministic dynamics for a colloid in a bath of small/fast solvent molecules to a stochastic model for the dynamics of the particle with the solvent represented only implicitly?

- Crooks fluctuation theorem with stochastic dynamics. What changes when you move away from Hamiltonian dynamics and into a stochastic dynamics like the Langevin dynamics discussed in the previous item?
- Renormalization and the Ising model. A powerful theoretical idea for analyzing phase transitions is called the renormalization group. You can show it off reasonably well with the one-dimensional Ising model. You can also see how/why it can become challenging to work with in the two-dimensional Ising model.

2. **A computational assignment.** Our final problem set, which will come out right before Thanksgiving, will explore phase transitions using a model of coupled spins known as the Ising Model. This model is very challenging to address with pencil and paper mathematics, but lots of insight can come from doing numerical calculations. In the problem set we will use Monte Carlo sampling methods (methods that use random chance as in the casinos in Monte Carlo) to see how an order parameter for the model can change very sensitively with external parameters (the temperature or the external magnetic field). Everyone will be carrying out the simplest part of the Monte Carlo sampling, but you can choose to continue with more complicated calculations for your final project. In particular, I'd ask you to use importance sampling techniques (as described in the first three sections of Chapter 6 in David Chandler's book) to compute the free energy of magnetization for a variety of temperatures and magnetic field strengths. If you think computations or simulations may be a significant part of your PhD research, this could be a good choice. The advantage is that I'll be writing something to walk you through the steps of what I'd like you to do, so it's a little less open-ended than the problem set question. The disadvantage is that you'll need to do some programming.